

Sandia H₂/He Flame: Scalar Data

Release 2.0 -- January 2003

Robert S. Barlow
Mail Stop 9051
Sandia National Laboratories
Livermore, CA 94551-0969
barlow@ca.sandia.gov
<http://www.ca.sandia.gov/TNF>

NEW IN RELEASE 2.0

Documentation file reformatted to PDF with added references. Scalar data archives updated to remove old documentation file. No changes to data or data descriptions.

NEW IN RELEASE 1.1b

Boundary conditions for H₂O in the coflow air had been labeled as mass fractions but values corresponded to mole fractions. This boundary condition is now listed correctly (in both units).

NEW IN RELEASE 1.1a

Axial profiles included for the undiluted and 20%-He cases. These were simply constructed from the r=0 data in the radial profiles.

NEW IN RELEASE 1.1

- 1) The archive SANDH2_A has been updated. SANDH2_B is unchanged.
- 2) The first release contained an error in the Favre-averaged fluctuations. This error has been corrected, and all the .fav files in SANDH2_A have been updated.
- 3) Files of conditional averages (.cnd files in SANDH2_A) have been updated to properly include the coflow air humidity for zero mixture fraction.
- 4) Mole fraction listings for all Reynolds-, Favre-, and conditionally-averaged results have been added. File descriptions are given below. Single-shot data are still given only in mass fractions.
- 5) A subscriber to the first release noted that the average mass fraction results show O₂ in the fuel-rich regions of some profiles. This may be an artifact caused by imperfect correction for the crosstalk of H₂ rotational Raman scattering onto the O₂ detector. It occurs only in some profiles and in limited ranges of mixture fraction, as may be seen in the scatter plots of mole fraction shown in Ref. [2]. In terms of mole fractions, the effect is very small. However, it is accentuated when results are considered as mass fractions, due to the high molecular weight of O₂ relative to the mean molecular weight of the mixture for fuel-rich conditions.

ABSTRACT

This file provides documentation for the Sandia data set of multiscale measurements in nonpremixed jet flames of H₂, 20% helium in H₂, and 40% helium in H₂. This data set includes simultaneous measurements of temperature, the major species mass fractions (O₂, N₂, H₂, H₂O), and the mass fractions of OH and NO, based upon the combination of spontaneous Raman scattering, Rayleigh scattering, and laser-induced fluorescence. The experimental procedures and many aspects of the data have been published in the references listed below. The full data set is available in electronic form from the web site of the *International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames* (<http://www.ca.sandia.gov/TNF>).

These scalar data are complemented by velocity measurements conducted at ETH Zurich. Consult the Workshop Web page listed above for information on the velocity data.

USE OF THE DATA

Please contact Robert Barlow at the above address if you use or publish these data. This will ensure that you will be on the mailing list for updates regarding these and other relevant data.

Any publications making use of these data should reference "R. S. Barlow, Sandia H₂/He Flame Data - Release 2.0, <http://www.ca.sandia.gov/TNF>, Sandia National Laboratories (2003)", as well as the two *Combustion and Flame* papers [2,3] that provide descriptions of the experiments.

NOTICE

This data release was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of the contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof or any of their contractors or subcontractors.

GENERAL DESCRIPTION OF THE FLAMES

A primary objective of this experimental series is to provide detailed information on thermal NO production in turbulent jet flames with relatively simple boundary conditions. Flow conditions are similar to those reported by Driscoll and Chen [1], who

made sampling probe measurements of NO and NO_x. The present data set includes radial profiles at several streamwise locations along the visible flame length for each of three flames: undiluted H₂, 20% He dilution, and 40% He dilution. Dilution reduces radiative loss, and in the most dilute case radiation has only a small influence on thermal NO production. In the context of model validation, dilution allows the effects of the radiation submodel to be isolated from turbulence, chemistry, and mixing submodels. Experimental results are discussed in [2,3], and some comparisons with predictions using Monte Carlo pdf and Conditional Moment Closure models have been published in [4,5,6]. LDV measurements at the same nominal flow conditions are available from ETH Zurich, and comparisons of the scalar/velocity data with Lagrange IEM and flamelet model predictions have been published [7]. Extensive comparisons of measured and modeled (Monte Carlo PDF and Conditional Moment Closure) results are reported in [8].

Radial profiles were obtained at several streamwise locations in each of the three flames. Typically, 500-800 samples were collected at each position. Flow conditions and measurement locations are given in Table 1. L_{vis} is the approximate visible flame length, L_{stoic} is the stoichiometric flame length based upon interpolation of results for the Favre average mixture fraction along the jet centerline, and the Reynolds numbers are calculated at the cold nozzle exit conditions using mixture viscosities from Chemkin. The Reynolds number for the 40% helium flame was reduced to avoid liftoff. Note that the Reynolds number for the 40% He case was printed in error in [2,3].

Table 1 Fuel Flow Conditions and Measurement Locations

H ₂ :He (by vol)	u _j (m/s)	Re _d	L _{vis} /d	Streamwise Locations (x/L _{vis})	L _{stoic} (mm)
100:0	296	10,000	180	1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 1	475
80:20	294	9,800	150	1/8, 1/4, 3/8, 1/2, 5/8, 3/4, 1	375
60:40	256	8,300	100	1/2, 3/4, 1	270

BOUNDARY CONDITIONS

The burner was a straight tube with a squared-off end (inner diameter, d=3.75 mm; outer diameter 4.84 mm). This was centered at the exit (30-cm by 30-cm) of a vertical wind tunnel contraction. The coflow air velocity was 1.0 m/s (±0.06 m/s), and the flames were attached and unconfined. Turbulence intensity has not been measured at this low coflow velocity. However, observation of laminar flames (Tsuji and jet geometries) in the facility suggest that coflow turbulence is insignificant for the present turbulent flame results. A free-stream turbulence intensity of 2% was measured at a higher mean velocity (40 m/s). The coflow air temperature was 294 K (±2K), and the humidity ratio in the coflow varied during the course of the experiments. Average values of the H₂O mole fraction and mass fraction in the coflow during measurements in each flame are listed below. It is important

to note that the ambient humidity affects NO production [8], and it should be included in model calculations of these flames.

H₂:He (by vol)	H₂O Mole Fraction in Coflow Air	H₂O Mass Fraction in Coflow Air
100:0	0.0115	0.0072
80:20	0.013	0.0081
60:40	0.013	0.0081

The fuel exit temperature was 295 K (± 2 K). Fully developed turbulent pipe flow may be assumed at the nozzle exit. Fuel flow velocities are given in Table 1.

EXPERIMENTAL UNCERTAINTIES

Measurement precision is limited primarily by shot noise in the Raman and LIF signals and by shot-to-shot variation in the lineshape of the flashlamp-pumped dye laser used for Raman/Rayleigh measurements. Table 2 includes the standard deviations of results in representative calibration flames. Table 2 also includes estimates of potential systematic errors that affect the accuracy of mean values of the measured scalars. These estimates are based on repeatability of Raman calibrations, changes in the Raman/Rayleigh laser characteristics during experiments, drift in the LIF dye laser wavelengths, and uncertainties in the fluorescence calibrations and corrections.

Table 2 Estimates of Experimental Precision and Accuracy

Scalar	%rms	phi	T (K)	Conc. (cm⁻³)	Systematic Uncertainty
N ₂	3.8	0.94	2350	2.1e+18	$\pm 3-4\%$
H ₂ O	4.8	“	“	1.0e+18	$\pm 3-4\%$
OH	7.5	“	“	2.2e+16	$\pm 15\%$
T	2.5	“	“	NA	$\pm 3\%$
F	5.1	“	“	NA	$\pm 3-4\%$
NO	12.5	0.5	1550	2.0e+13	$\pm 15-20\%$

The uncertainties listed are representative of conditions near the stoichiometric mixture fraction (approximately $0.5 < F/F_{\text{stoic}} < 2.0$). Due to limitations in the calibration procedures, the uncertainties may be greater for very rich samples and for lean samples having intermediate temperatures (approximately 400 K to 1000 K). This is because the Raman system response functions for this temperature range were based on interpolation between calibrations at room temperature and accessible flame temperatures.

Preferential diffusion of helium may cause errors in the results that cannot be estimated from the calibration procedures. The helium concentrations are not measured (no Raman scattering signal from helium), but rather must be calculated from the elemental hydrogen balance, based upon the assumption of equal mass diffusivities. Helium will tend to diffuse faster than H₂O, leading to excess helium mole fractions in fuel-lean samples.

This could cause an upward bias in the Rayleigh temperature measurements in fuel-lean samples. Comparisons with model predictions of conditional mean temperatures have given some indication of this phenomenon. However, it does not appear to be a large effect.

DIFFERENCES BETWEEN THE THESE LISTINGS AND PREVIOUSLY PUBLISHED DATA

There are minor differences between the present listing and the originally published results for these flames. First, the present listing includes the mixture fraction calculated according to the formulation given by Bilger. (See Ref. [2] for the definition used previously.) Second, the present data reduction process no longer includes an estimate of the H-atom concentration in the quenching corrections for NO. Differences resulting from these changes are small compared to the experimental uncertainties in mixture fraction and NO concentration.

FILE NAMES AND FILE FORMATS

Data file names use the following system to indicate the flame, location, and type of data in the file. There are three types of averaged data files and two types of files that include single shot data.

Example file name: he2x34.ave
 -----.

Flame type
 he0 - 0% helium (undiluted H₂)
 he2 - 20% helium
 he4 - 40% helium

Axial location
 x18 - $x/L_{vis} = 1/8$
 x14 - $x/L_{vis} = 1/4$
 x38 - $x/L_{vis} = 3/8$
 x12 - $x/L_{vis} = 1/2$
 x58 - $x/L_{vis} = 5/8$
 x34 - $x/L_{vis} = 3/4$
 x11 - $x/L_{vis} = 1$

Data type (Extension)
 .ave - radial profile of ensemble averages (mean and rms)
 .fav - radial profile of Favre averages (mean and rms)
 .cnd - conditional averages (mean and rms) of all data at
 that axial location
 .cmp - composite file of 1000-2000 single-shot data from
 several locations in a radial profile. These are
 for generating scatter plots. 50 to 300 points
 are included from each radial position, and the
 radius is tabulated for each point.
 .sct - all single-shot data from a fixed location.

The file names for the .sct files include two additional digits that indicate radial location in (mm). For example: he0x3415.sct contains single-shot data from the undiluted flame, axial location of $x/L_{vis}=3/4$, radial location of $r=15$ mm. In forming the file names the radial location is rounded up to the nearest integer value. The actual location is included in the file header.

Data are distributed in two archives (compressed in formats for Windows and Unix platforms). The first archive contains the .stat and .cmp files, which will be sufficient for most comparisons with model predictions. The second archive contains all .sct files, which will only be needed if pdf's are to be extracted or additional statistical analysis is to be done. The directory structure for the archives is:

SANDH2_A

SandH2He - main directory

SandH2He.pdf - documentation file

he0 - subdirectory for the undiluted flame

he0cmp - subdirectory with .cmp files (mass fractions only)

he0statY - subdirectory with .ave, .fav, and .cnd files for mass fractions

he0statX - subdirectory with .ave, .fav, and .cnd files for mole fractions

he2 - subdirectory for the 20% helium in H2 flame

he2cmp - subdirectory with .cmp files (mass fractions only)

he2statY - subdirectory with .ave, .fav, and .cnd files for mass fractions

he2statX - subdirectory with .ave, .fav, and .cnd files for mole fractions

he4 - subdirectory for the 40% helium in H2 flame

he4cmp - subdirectory with .cmp files (mass fractions only)

he4statY - subdirectory with .ave, .fav, and .cnd files for mass fractions

he4statX - subdirectory with .ave, .fav, and .cnd files for mole fractions

Note: File names for mass fractions and mole fractions are the same. Only the subdirectory names are different.

SANDH2_B (mass fractions only)

SandH2He.pdf - documentation file

he0sct - directory with .sct files

(all single-shot data from undiluted H₂)

he2sct - directory with .sct files

(all single-shot data from 20% He in H₂)

he4sct - directory with .sct files

(all single-shot data from 40% He in H₂)

All data files are ASCII text files with columns separated by 1 or more spaces. Column labels are included in all files. Listings include:

Fblgr - The Bilger mixture fraction defined from hydrogen and oxygen elemental mass fractions as,

$$\text{Fblgr} = \frac{0.5(YH-Y2H)/WTH - (YO-Y2O)/WTO}{0.5*(Y1H-Y2H)/WTH - (Y1O-Y2O)/WTO}$$

where

YH = H element mass fraction in the measured sample

YO = O element mass fraction in the measured sample

Y1H = H element mass fraction in fuel stream

Y1O = O element mass fraction in fuel stream

Y2H = H element mass fraction in coflow stream

Y2O = O element mass fraction in coflow stream

and WTH = 1.008, WTO = 16.0

T(K) - The temperature determined from the Rayleigh scattering signal and a species weighted Rayleigh cross section based on mole fractions from the Raman measurements of major species. Radicals and Ar from the air are not included in determining the Rayleigh cross section of the mixture, and the resulting temperature error is negligible compared to the quoted temperature uncertainty.

Species Mass fractions - O₂, N₂, H₂, H₂O, OH, and NO mass fractions are reported. The sum is normalized to unity, even though some minor species are not measured. Helium is included in the mass fraction calculation for the dilute flames but is not tabulated. The helium mass is determined assuming no differential diffusion of He and the hydrogen containing species.

NO mole fraction (XNOppm) is listed in addition to mass fraction, because NO levels are often quoted in ppm.

TNDR - This is defined as the ratio of total number densities determined from Raman/LIF and Rayleigh measurements. Equivalently, TNDR is equal to the ratio of temperatures determined from Rayleigh and Raman measurements.

$$\text{TNDR} = (\text{Raman/LIF Number Density}) / (\text{Rayleigh Number Density})$$

$$\text{TNDR} = (\text{Rayleigh temperature}) / (\text{Perfect Gas Temperature from Raman/LIF data})$$

In these measurements the temperature determined from Rayleigh scattering is considered to be more accurate than the temperature determined using the perfect gas law and the total number density of measured species. TNDR is tabulated with the single-

shot data to allow the original species concentrations to be recovered from the mass fractions. Shot noise will cause TNDR to differ from unity for single-shot measurements. Calibration uncertainties, including changes in laser lineshape, can also cause TNDR to differ from unity in single-shot and averaged results. Ensemble-average and conditional-average results for TNDR are tabulated in the .ave and .cnd files.

For most files the average value of TNDR is within a few percent of unity, indicating good agreement between the two temperature measurements. However, larger average values occur in the data for the undiluted flame at streamwise locations $x/L_{vis}=1/2$ and $x/L_{vis}=1$, which were taken on a separate day and appear to suffer more from drift in the calibrations. Modelers are advised to be more cautious of these files.

REFERENCES

1. Driscoll, J. F., Chen, R.-H., Yoon, Y., *Combust. Flame* 88:37-49 (1992).
2. Barlow, R. S. and Carter, C. D., *Combust. Flame* 97:261-280 (1994).
3. Barlow, R. S. and Carter, C. D., *Combust. Flame* 104:288-299 (1996).
4. Smith, N.S.A., Bilger, R.W., Chen, J.-Y., *Proc. Combust. Inst.* 24:263 (1992)
5. Smith, N.S.A., Bilger, R.W., Barlow, R.S., Carter, C.D., J.-Y. Chen, *Combust. Sci. Technol.* 105:357, (1995).
6. Chen, J.-Y., Chang, W.-C., Koszykowski, M., *Combust. Sci. Tech.* 110-111:505-529 (1995).
7. Schlatter, M., Ferreira, J., C., Flury, M, Gass, J., *Proc. Combust. Inst.* 26:2215 (1996).
8. Barlow, R. S., Smith, N. S. A., Chen, J.-Y., and Bilger, R. W., *Combust. Flame* 117:4-31 (1999)